


Next-Generation Scientists and Engineers Tap Lab's Resources

*A Livermore
fellowship program
provides students
practical experience
while they earn
their doctorates.*

THIS year, approximately 12,750 science and engineering students are enrolled in doctoral programs at the 10 University of California (UC) campuses. The academic requirements they must fulfill include researching and writing a thesis in their chosen field. About 50 fortunate students have been granted fellowships for up to four years to conduct research at the Laboratory using some of the most advanced facilities in the world while earning their Ph.D.s. This select group participates in Livermore's Student Employee Graduate Research Fellowship (SEGRF) Program.

The SEGRF Program traces its roots to the UC Davis Department of Applied



University of California (UC) at Davis student Erica McJimpsey works on one of the Laboratory's bioaerosol mass spectrometers.

Science (DAS), which was established at the Laboratory by Livermore cofounder Edward Teller in 1964. With a life-long commitment to science education, Teller recognized the need for a graduate program in applied science. He worked with UC administration to site a university-level education facility at the Laboratory and served as the first administrator of DAS. The SEGRF Program has supported students at DAS.

Over the years, graduate education opportunities at Livermore have grown to be broader than the disciplines emphasized in DAS. In 1999, the SEGRF Program opened to all UC Davis departments to meet the Laboratory's need for graduate students in areas such as laser physics, plasma diagnostics, fusion energy, accelerator technology, computational sciences, biosciences, materials science, and environmental and energy sciences. In 2001, the program opened to all UC campuses.

To apply for the SEGRF Program, students must pass their preliminary exams for Ph.D. candidacy, propose a project of interest to the Laboratory, and have a university thesis advisor and a

Laboratory mentor. SEGRF recipients are selected from a pool of applicants by a committee of representatives from all of the Laboratory's directorates. In support of the directorates, Livermore's University Relations Program (URP) manages the SEGRF Program and facilitates interactions with UC campuses.

Paul Dickinson, who manages the SEGRF Program at Livermore, says, "To maintain the Laboratory's scientific and technological excellence, it is essential that we recruit bright, young scientists and engineers." SEGRF participants are half-time Laboratory employees during the academic year and full-time employees over the summer.

The program has achieved impressive results. Forty-five percent of SEGRF students become Laboratory employees. "Many of the other students go to other national laboratories or universities and collaborate with us on projects or become a resource for recruiting other students," says Dickinson.

Cornucopia of Experts

The Laboratory's longtime approach of using multidisciplinary collaborations to solve problems benefits the SEGRF Program. Erica McJimpsey, a UC Davis student and SEGRF participant, says, "I'm working with a team of engineers, biologists, computer scientists, physicists, and chemists, which is an advantage I wouldn't have in an academic environment." For her Ph.D. in analytical chemistry, McJimpsey is writing a dissertation on the characterization of single-particle ionization. She is working with the Laboratory's Bioaerosol Mass Spectrometry Group within the Chemistry and Materials Science Directorate.

In 2001, a Livermore team, originally funded by the Laboratory Directed Research and Development (LDRD) Program, developed the bioaerosol mass spectrometry (BAMS) system—the only instrument that can distinguish between two related but different spore species in less than 1 minute. The mass spectrometer

UC Berkeley student Ionel Dragos Hau (right) holds a lithium fluoride crystal similar to one he and his Laboratory mentor Stephan Friedrich (left) are using for a neutron spectrometer (forefront).



can also sort out a single spore from thousands of other particles. (See *S&TR*, September 2003, pp. 21–23; October 2005, pp. 8–9.) The BAMS team won a 2005 R&D 100 Award from *R&D Magazine* for developing the instrument. The Department of Defense's (DoD's) Technical Support Working Group and Defense Advanced Research Project Agency funded the Livermore team to develop BAMS for its potential use in identifying biological agents such as anthrax.

McJimpsey is working with the team to extend the spectrometer's capability for identifying signatures of proteins in individual spores. The team is using an ionization technique called matrix-assisted laser desorption ionization (MALDI) to analyze single particles and achieve greater sensitivity. In MALDI, the biomolecule of interest, often a protein, is irradiated with a laser. Because proteins are sensitive to temperature changes and can easily degrade, a chromophore (a molecule that absorbs light) is mixed with the protein to absorb the brunt of the energy from the laser.

Livermore has three BAMS instruments, one of which was modified by McJimpsey and two former SEGRF students, Scott Russell and Gregg Czerwieniec, to conduct the experiments using the MALDI technique. "At the Laboratory," says McJimpsey, "I can apply my passion for instrumentation toward an important homeland security mission." In addition to her professional goal of obtaining a DoD Presidential Management Internship to work on homeland security, McJimpsey also hopes to be a role model and mentor to minorities interested in pursuing careers in science.

In another homeland security effort, Ionel Dragos Hau, a nuclear engineering student at UC Berkeley and SEGRF participant, is working with Livermore's Advanced Detector Group to develop a novel type of neutron spectrometer as part of his thesis on neutron detection. One advantage of this neutron spectrometer is



Laboratory postdoctoral researcher Faranak Nekoogar conducts research in ultrawideband radio-frequency identification systems.

that its sensitivity is so high it can detect light elements, such as oxygen, within a heavy matrix such as plutonium. It can also detect nuclear material behind a heavy metal that would shield other types of radiation such as gamma rays. For example, if nuclear material were concealed in a lead object, the material's neutrons would interact with the lead and scatter in ways that provide a signature identifiable to the neutron spectrometer. The team uses lithium fluoride for the detector material because large crystals of it can be grown; the greater the size of the crystal, the greater the capability to detect neutrons.

Unlike spectrometers that collect electrical charges, this neutron detector collects heat in the form of phonons produced from a neutron reaction. A thermometer measures the rapid increase in heat, and the source of the nuclear material is revealed by the strength of the heat signal. However, because the heat has to flow out of the detector after each neutron interaction before another count

can be taken, and phonons travel more slowly than electrons, the count rate is comparably lower than some types of gamma-ray detectors. Hau is working with the Livermore team to improve the spectrometer's count rate.

Researchers, Authors, and Inventors

Livermore scientists and engineers benefit from the students' intellectual vitality and the fundamental research they conduct. The students greatly contribute to work that is publishable in papers, an important part of both the student's and the Laboratory scientist's career development. Some of the SEGRF students are well-seasoned authors by the time they complete their Ph.D.s. In addition to publishing articles on ultrawideband (UWB) communications, former SEGRF student Faranak Nekoogar, now a postdoctoral researcher in the Engineering Directorate, published two technical books and filed eight patents or records of inventions before completing her Ph.D.

UWB communication is fundamentally different from conventional communication systems because it employs extremely narrow (picoseconds to nanoseconds) radio-frequency pulses to communicate between transmitter and receiver. (See *S&TR*, September 2004, pp. 12–19.) Using short-duration pulses rather than continuous waveforms offers several advantages over traditional wireless technologies. They include large throughput, covertness, tamper-resistance to jamming, low transmit power, and the ability to coexist with current radio services.

A very low-power UWB radar system called micropower impulse radar (MIR) was invented in 1993 by Livermore electronics engineer Tom McEwan. It has been one of the most commercially successful licensed inventions both at Livermore and throughout the Department of Energy (DOE). Livermore won R&D 100 awards for two of the technologies that use MIR—an electronic dipstick (*S&TR*, October 1996, pp. 16–17) and a bridge inspection system (*S&TR*, October 1998, pp. 7–8). The Laboratory holds 30 MIR patents and patent filings, with Nekoogar's among them.

UWB pulses are safe to use around people and do not interfere with computers, digital watches, cellular phones, or radio and television signals. UWB technology could replace the interface between computers, printers, and entertainment devices in homes, providing a wireless network of integrated systems. Nekoogar says UWB technology could also overcome the power and range limitations of the current radio-frequency identification systems, providing more reliable monitoring of assets and people. In addition, it has potential use in tracking applications to prevent cargo-container tampering, provide situational awareness for soldiers, and help find lost children.

DoD and the Department of Homeland Security are interested in UWB technology for covert communications in mission critical applications. Nekoogar wrote her thesis on the use of UWB transmitted-reference (TR) methods that enable reliable wireless communications in harsh radio propagation conditions. For example, in the heavy metallic environment inside a ship, where conventional wireless technologies fail because multiple reflections of radio signals interfere with each other.

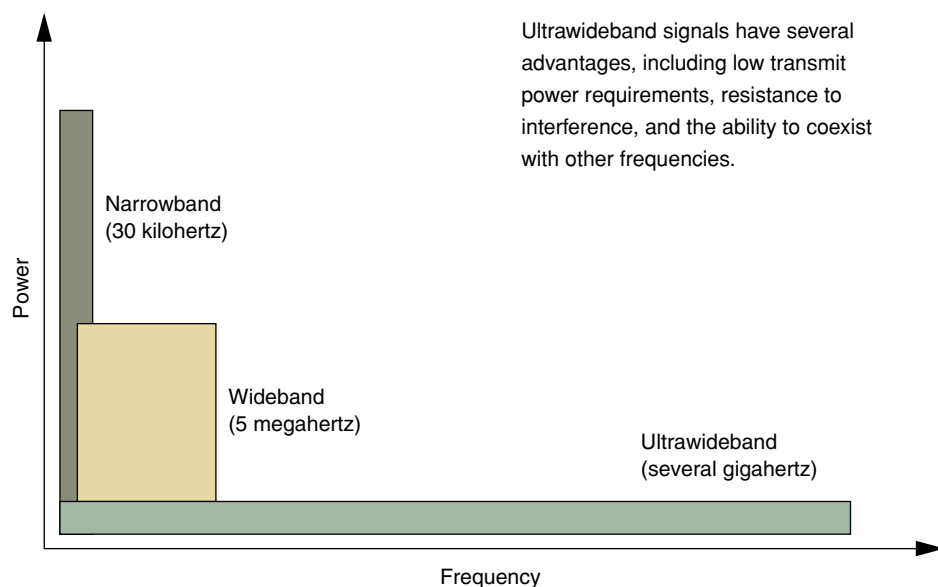
Nekoogar says the next step will be designing chips to carry UWB-TR systems. “We want to partner with industries that specialize in chip design.” Chip design is the subject of the second book Nekoogar has authored; her first book describes the fundamentals of UWB communications.

Partnering with Industry

SEGRF students also have opportunities to partner with industry. As part of Nick Killingsworth's thesis on combustion control in homogenous charge compression ignition (HCCI) engines, the UC San Diego student works with Livermore engineers on an HCCI engine. “I had been studying HCCI technology at UC San Diego and, in particular, combustion control issues,” says Killingsworth. “One day, I received an advertisement about the SEGRF Program. It was perfect timing. I contacted the Livermore team right away.”

Caterpillar Inc. donated a six-cylinder, spark-ignited (SI) engine, which the Livermore team is converting to an HCCI engine in exchange for providing the company with research data. (See *S&TR*, April 2004, pp. 17–19.) The research is funded by the California Energy Commission's Advanced Reciprocating Internal Combustion Engine Program and DOE's Office of Energy Efficiency and Renewable Energy.

Combustion in HCCI engines is fundamentally different from that in SI and diesel engines. HCCI combustion involves thermal auto-ignition of a premixed fuel–air mixture, without the flame propagation found in SI engines or the mixing-controlled combustion found in diesel engines. HCCI engines can run extremely lean (low percentage of fuel and a high percentage of air), and the combustion temperature is low enough that the engine produces extremely low nitrogen oxide emissions (a few parts per million). Lean, premixed combustion also results in nearly zero particulate matter emissions.



However, HCCI engines present challenges that have kept them from commercialization. The main hurdles are combustion-timing control, low power output, and difficulty in starting when cold. At cold start, the compressed-gas temperature in an HCCI engine is low because the charge receives no preheating from the intake manifold and the compressed charge is rapidly cooled by heat transfer to the cold combustion chamber walls.

The Livermore team's novel solution is to start the engine directly in HCCI mode by preheating the intake with a gas-fired burner. Running the intake charge through the preheater while simultaneously spinning the engine with an air starter enables the HCCI engine to achieve ignition. After ignition, the combustion is self-sustaining, and the burner can be turned off.

Combustion-timing control, particularly under a range of speeds and loads, is the most challenging problem.

The HCCI engine does not have a combustion trigger such as a spark plug or fuel injector. Instead, combustion is achieved by controlling the temperature, pressure, and composition of the fuel-air mixture. Multiple-cylinder engines pose an additional challenge because differences in pressure, temperature, and compression ratio invariably exist between the cylinders.

To address this problem, the Livermore team developed a thermal management system in which a controller detects

cylinder-to-cylinder differences and adjusts the intake temperature of each cylinder for optimal combustion timing. Killingsworth is developing the control algorithms to regulate the opening and closing of the cylinders' valves.

The team plans to use the engine as a test bed for HCCI studies. HCCI technology can considerably improve fuel efficiency while providing unmatched flexibility in operating temperatures. At the same time, the technology will meet the stricter

UC San Diego student Nick Killingsworth (center) and his Laboratory mentors Daniel Flowers (left) and Salvador Aceves (right) are converting a Caterpillar spark-ignited engine to a homogenous charge compression ignition engine.



California standards for nitrogen oxide emissions, which go into effect next year.

Combining Talent for a Common Goal

Occasionally, former and present SEGRF students work together as a research team. Physicists Wren Carr and John Adams, both former SEGRF students and now Laboratory employees, are working with UC Davis SEGRF participant Paul DeMange. The team is conducting research relevant to the National Ignition Facility (NIF), the world's most energetic laser being constructed for the National Nuclear Security Administration's Stockpile Stewardship Program. (See *S&TR*, September 2002, pp. 20–29.)

DeMange is investigating the fundamental processes associated with laser-induced damage in optical materials. His experiments have already led to five coauthored publications in journals such as *Applied Physics Letters* and *Optics*

Letters. Many of DeMange's research experiments were performed using new instruments that he and Carr built to provide rapid, quantitative measurements of the density of damage sites in crystals.

DeMange's early experiments investigated the effects of using different wavelengths to condition potassium dihydrogen phosphate crystals such as those used in NIF. Conditioning is the process of increasing a crystal's resistance to laser-induced damage by pre-exposing the crystal to subdamaging laser intensities. DeMange's results showed that the effectiveness of conditioning is sensitive to the wavelength of the laser light used, with shorter wavelengths providing a better level of conditioning. He also confirmed that exposure to two pulses of different wavelengths simultaneously resulted in more damage than that resulting from exposure to each wavelength separately.

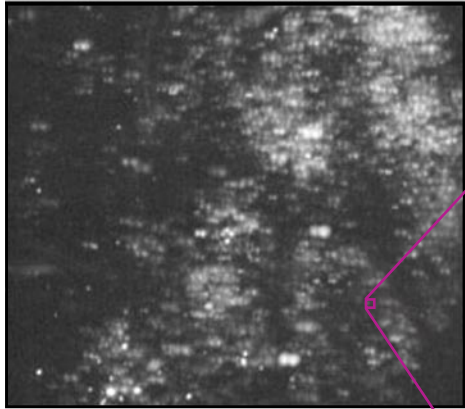
Adams received his Ph.D. through DAS in 2002. While a SEGRF student, he discovered a widely tunable midinfrared laser material that has potential applications for remote sensing of a variety of atmospheric-borne chemicals. He also discovered a new electrooptic material for use at wavelengths near 1 micrometer, for which he earned a patent, and a new frequency-conversion material. Adams recalls being struck by the wealth of knowledge available to him as a student. "The Laboratory is so full of top-notch people that I can't imagine a better environment for a budding Ph.D. If I had a question while reading a journal article, I could often walk down the hall and ask the lead author for clarification. Or, if a piece of equipment broke, an expert was always around to help me. To have access to these resources as a student was phenomenal."

Adams and DeMange's studies are providing Carr with data he needs as

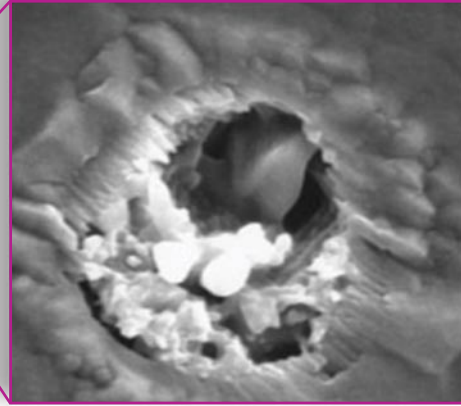
Laboratory physicists Wren Carr (center) and John Adams (right) collaborate with UC Davis student Paul DeMange (left) on the investigation of laser-induced damage in optical materials for the National Ignition Facility.



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A scanning electron microscope image of a crystal shows the damage imprint left by a laser beam.



principal investigator for a \$1.5 million LDRD project studying conditioning in crystals to mitigate laser-induced damage. Carr says, "Part of the purpose of the LDRD effort is to better understand the laser parameters that govern conditioning of crystals." His work has focused on studying the mechanisms involved in energy deposition by low-intensity, visible, and near-ultraviolet laser light in a material, the mechanisms that govern laser-induced damage, laser machining, and laser conditioning.

While a SEGRF student, Carr demonstrated that damage induced by a laser pulse a few nanoseconds long results in a tiny region inside the crystal reaching a temperature of 12,000 kelvins and a pressure of 250,000 atmospheres of pressure, far higher than had been theorized. The damage sites, which are only a few micrometers in diameter, were examined using a scanning electron microscope and were found to have the same general structure of craters made by underground explosions with 20 orders of magnitude more energy.

Are Diamonds Really Forever?

Laser-induced damage in optical materials is one example of modifications that result from extreme conditions. Studying materials exposed to extreme conditions often requires the use of simulations. SEGRF students have

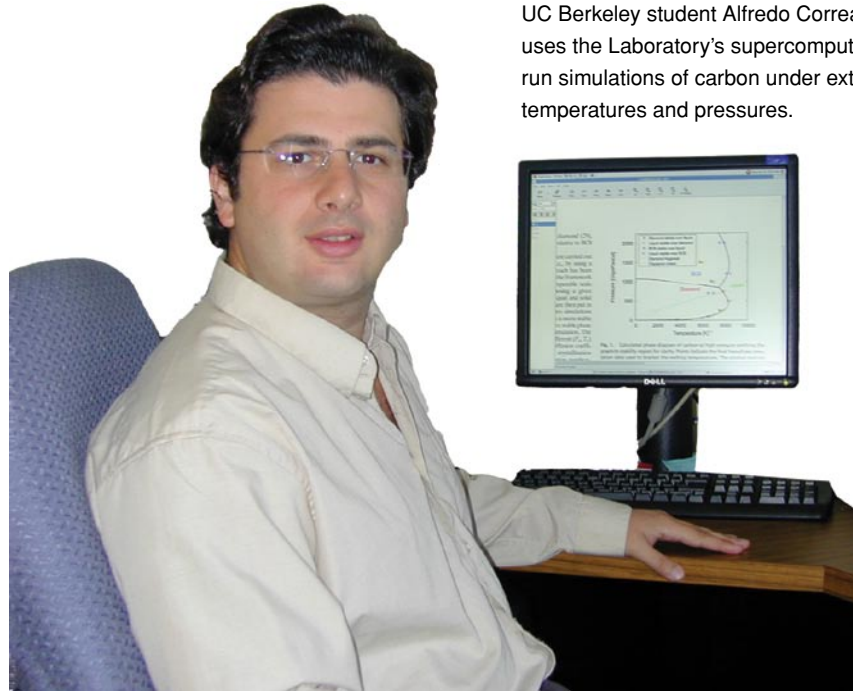
opportunities to conduct research using some of the fastest supercomputers in the world. Alfredo Correa-Tedesco, a theoretical physics student at UC Berkeley, uses the Laboratory's 11-teraops (trillion operations per second) Multiprogrammatic Capability

Resource (MCR) and 23-teraops Thunder machines to run three-dimensional simulations of carbon at high pressures and temperatures. Correa-Tedesco's work is part of a study to determine carbon's phase diagram.

Carbon is one of the most abundant elements in the universe. In its elemental form, carbon is found in coal, graphite, diamond, bucky balls, and nanotubes. These are materials with very different properties, yet at the microscopic level, they differ only by the geometric arrangements of atoms. Little is known about the phase boundaries and melting properties between different crystalline phases of carbon and liquid carbon. Experimental data are scarce because of difficulties in reaching a million atmospheres of pressure and thousands of kelvins in the laboratory.

Correa-Tedesco uses Qbox, a first-principles code developed by physicist Francois Gygi, formerly at Livermore and now at UC Davis. Qbox can simulate hundreds of atoms at a time

UC Berkeley student Alfredo Correa-Tedesco uses the Laboratory's supercomputers to run simulations of carbon under extreme temperatures and pressures.



and allows the team to model the transition between two phases in a single simulation cell. “Modeling the coexistence of two phases is difficult,” says Correa-Tedesco. “We need the supercomputing capabilities of MCR and Thunder. It takes three to four days and 400 processors of MCR for results, but it could take a year or more for such a simulation without them.”

The team determined the solid–liquid and solid–solid phase boundaries of carbon for pressures up to 20 million atmospheres and more than 10,000 kelvins. “We expected to determine just the melting transition for one solid phase,” says Correa-Tedesco. “Instead, we found the melting transitions for two solid phases of carbon and the transition between two phases of solid.” The results will help researchers devise models of Neptune and Uranus, including an estimate of the planets’ core temperatures.

The results will also provide valuable data for experimental studies used to characterize materials at extreme pressures. One of the experimental methods involves using a diamond anvil cell (DAC), which is a small mechanical press that forces together two brilliant-cut diamond anvils.

(See *S&TR*, December 2004, pp. 4–11.) The diamond tips press on a microgram sample of a material to create extremely high pressures. Diamonds are used because they are the hardest known solid and can withstand ultrahigh pressures. They also permit x rays and visible light to pass unhampered through their crystalline structure.

Because diamond is a form of carbon, understanding phase transitions of carbon provides insight on diamonds used in DAC. “Experimentalists are interested in knowing the limits of diamond, for example, at what temperature and pressure the diamond will be destroyed,” says Correa-Tedesco. “They also want to know other characteristics about diamond, such as whether it becomes conducting at high temperatures.”

The team discovered that diamond remains insulating—that is, resistant to the movement of its electrons—in the solid phase, while it metallizes at melting. Under extreme pressures, certain electrons, which are normally tightly held within an atom’s inner electron bands or shells, can move about, resulting in changes in material properties and molecular structures. The

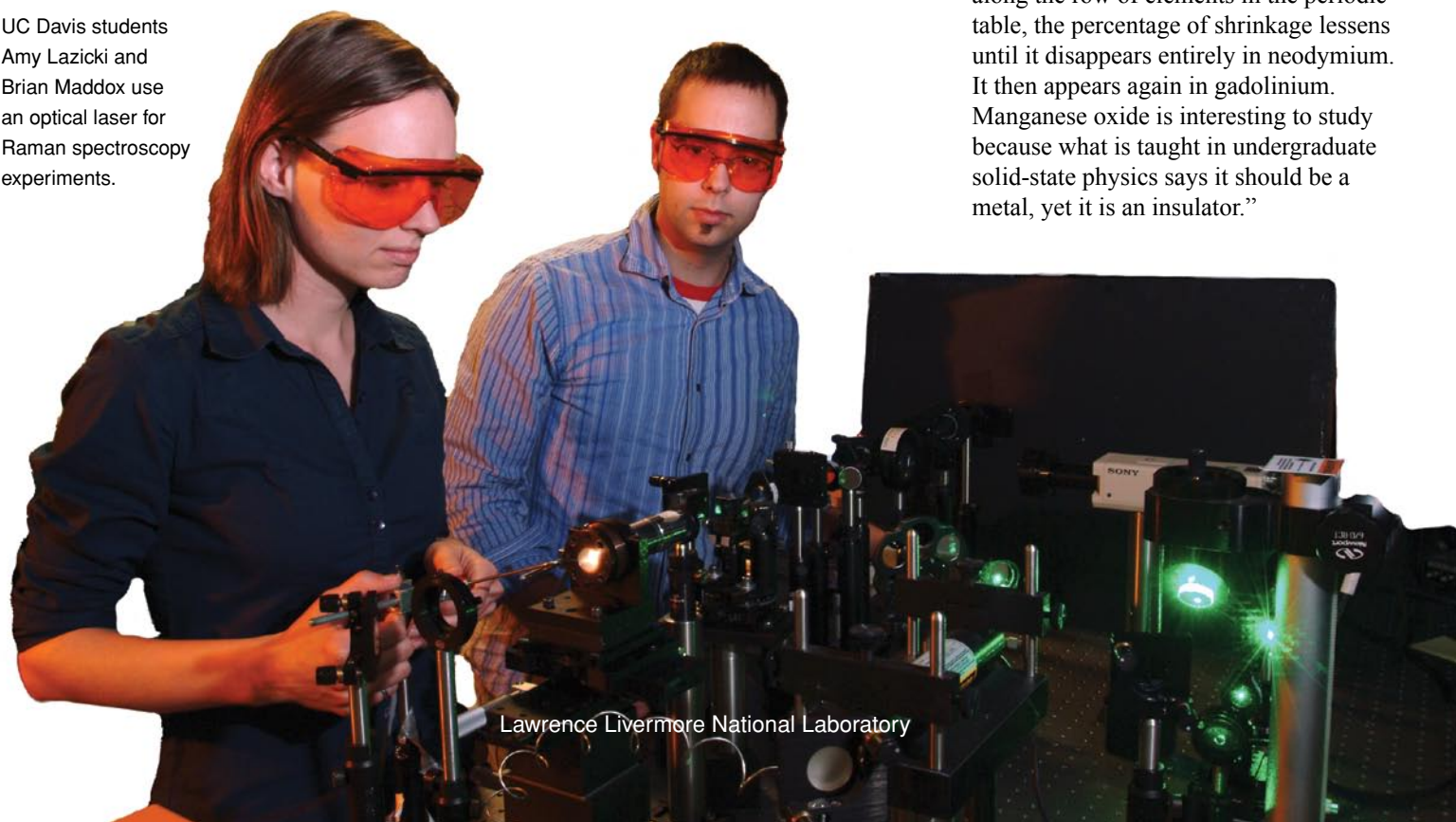
transition is marked by a reduction in the sample’s volume as the crystalline lattice shifts to accommodate the new electronic configuration.

Resolving Theoretical Mysteries

Two SEGRF students from UC Davis, Brian Maddox and Amy Lazicki, are combining a DAC with x-ray diffraction techniques to study the effects of pressure on the electronic structure of certain materials during the phase transitions. Maddox works in the Physics and Advanced Technologies Directorate studying transition metal compounds, such as manganese oxide, and rare-earth metals, such as the lanthanides cerium, gadolinium, and praseodymium, all of which exhibit large volume collapses at high pressure. The lanthanides are important to study because the same volume shrinkage occurs in the actinides, which are the elements belonging to the row in the periodic table below the lanthanides and include the nuclear weapon metals plutonium and uranium.

Maddox says, “When we apply pressure to cerium, its volume shrinks by about 17 percent. However, the structure of the material doesn’t change. As we move along the row of elements in the periodic table, the percentage of shrinkage lessens until it disappears entirely in neodymium. It then appears again in gadolinium. Manganese oxide is interesting to study because what is taught in undergraduate solid-state physics says it should be a metal, yet it is an insulator.”

UC Davis students Amy Lazicki and Brian Maddox use an optical laser for Raman spectroscopy experiments.



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One of the theories to explain the volume shrinkage is the Mott transition theory. The theory proposes that pressure could drive manganese oxide from its anomalous insulating state to a metallic state. Until the invention of the DAC, experimental methods for detecting this type of transition of a substance at high pressure were not available. Maddox's experiments may help determine if the Mott transition theory is correct.

Maddox conducts his experiments using elastic x-ray scattering techniques, such as angle-dispersive x-ray diffraction (ADXRD), and inelastic x-ray scattering techniques, such as x-ray emission spectroscopy and resonant inelastic x-ray scattering. For many years, researchers have conducted inelastic scattering experiments on large samples at room temperature. However, until advancements were made in the synchrotron—a particle accelerator that boosts the velocity of electrons to nearly the speed of light—the techniques could not be applied to high-pressure samples inside a DAC. In ADXRD experiments, researchers send a beam of highly focused x rays through a sample in the DAC and record the diffraction pattern on an image plate detector, which is sensitive to x rays. Changes in the diffraction pattern reveal how a material's structure responds to pressure. Maddox used the synchrotron at Argonne National Laboratory's Advanced Photon Source (APS) to conduct his experiments on manganese oxide. The results showed a transition at

300 kelvins and 1.07 million atmospheres of pressure. "These results confirmed that the compound exhibits similarities to transitions in the lanthanides and actinides as has been predicted," says Maddox.

Lazicki also uses the APS synchrotron and a DAC to conduct ADXRD and x-ray Raman spectroscopy experiments on lithium compounds, such as lithium oxide and lithium nitride, which are analogs to hydrogen-containing materials. X-ray diffraction techniques, including ADXRD, require more than one electron to map the position of an atom's electrons. Hydrogen has only one electron, so researchers often use hydrogen's nearest neighbor lithium, which has three electrons, to further their understanding of the nature of hydrogen compounds.

The team's results for lithium nitride showed the first experimental evidence that this compound undergoes a phase transition near 395,000 atmospheres of pressure. "The transformation represents a state that is uncommonly stable and compressible up to at least 2 million atmospheres of pressure," says Lazicki. "Lithium nitride is also one of the most difficult materials to metallize, with the metallization transition predicted to occur at 80 million atmospheres of pressure."

Maddox notes that although he works with an experimental group at Livermore, his advisors at Davis are theoretical physicists working on computational models. Maddox and Lazicki's data are useful feedback for their studies.

Maintaining Vision of Excellence

Over the years, the SEGRF Program has provided hundreds of young scientists and engineers a springboard to their professional careers. In exchange, the students have helped vitalize the Laboratory's research efforts and conducted studies of important fundamental science.

After graduation, many of the students remain at Livermore to contribute toward its national security missions. Dickinson notes, "The program has proven to be an important recruiting vehicle for building and maintaining scientific and engineering excellence at Livermore."

—Gabriele Rennie

Key Words: bioaerosol mass spectrometry (BAMS) system, Department of Applied Science (DAS), diamond anvil cell (DAC), homogenous charge compression ignition (HCCI), matrix-assisted laser desorption ionization (MALDI), neutron spectrometer, potassium dihydrogen phosphate, Qbox, Student Employee Graduate Research Fellowship (SEGRF) Program, ultrawideband (UWB) communications.

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